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ORGANIC COMPOUNDS IN TURBINE COMBUSTOR EXHAUST.(U)

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Trace organic compounds in aircraft turbine combustor exhaust were determined as functions of fuel type and engine operating pressure (power setting). Hydrocarbons were collect~~ion was done~~ed by multi-stage cryogenic sampling. Chemicals were analyzed ~~characterization was accomplished~~ by a coupled gas chromatograph-mass spectrometer-data system. Results ~~were~~ are presented in the context of assessment of biomedical impact of aircraft operations.

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ORGANIC COMPOUNDS IN TURBINE COMBUSTOR EXHAUST

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Abstract

Trace organic compounds in aircraft turbine combustor exhaust were determined as functions of fuel type and engine operating pressure (power setting). Hydrocarbons were collected by multistage cryogenic sampling. Chemicals were analyzed by a coupled gas chromatograph-mass spectrometer-data system. Results are presented in the context of assessment of biomedical impact of aircraft operations.

Introduction

Assessment of the biomedical impact of aircraft operations requires detailed information of the exhaust hydrocarbons related to both fuel type and engine operation conditions. To assess the toxic hazard potential of aircraft operations on ground personnel, the United States Air Force School of Aerospace Medicine (USAFSAM) and the Air Force Aero Propulsion Laboratory (AFAPL) have conducted a continuing cooperative study to investigate the hydrocarbon constituents in turbine engine combustor exhaust. Two reports of previous endeavors have been made since initiation of the program in late 1972[1,2]. This study has used long-term, on-line exhaust sampling with an improved version of the USAFSAM cryogenic trapping system[3]. The collected samples were analyzed with a coupled gas chromatograph-mass spectrometer-data (GC-MS-DATA) system.

This report details the results from the third sampling test, conducted in March 1975, to identify and quantitate hydrocarbon emissions from the T-56 combustor as a function of fuel type and combustor operating inlet pressure. The T-56 engine is of the turbine-driven propeller type (turboprop) used on the Air Force C-130 transport aircraft.

Experimental

Test Parameters

A single T-56 combustor installed in equipment that simulates the airflow and fuel ratio characteristics of an actual engine was provided in the AFAPL combustor rig. Compressors and a nonvitiated heating system supply air at appropriate temperatures, pressures, and flow rates for the series of tests.[4]

The fuels used were JP-4, JP-5, JP-8, DEL-5, and isooctane. The JP-4 was tested at inlet pressures of 15, 33, and 50 psig, which corresponds to low-, mid-, and high-pressure-ratio (PR) idle respectively. JP-8, isooctane, JP-5, and DEL-5 (an alternate fuel blend which might be produced from coal or a marlstone-type inorganic component mixed with an organic polymer kerogen, oil shale[5] were tested at mid-PR idle. Additionally JP-5 and JP-5/ferrocene blend were tested at simulated high power conditions.

Sampling

The combustor exhaust was continously sampled from a water-cooled orifice (1.1-cm) probe opening on the centerline of the combustor located approximately 10 cm behind the combustor exit. The 20-ft (6.1-m) line from the probe to the takeoff to the cryogenic trapping system was maintained at a temperature range of 90-200°C (Fig. 1). A 3-m-long .64-cm thick walled teflon line connected the takeoff point to the USAF cryosampler.

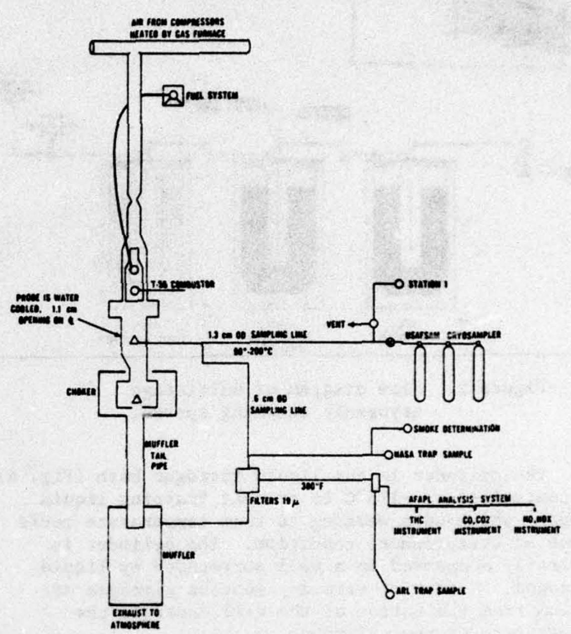

Figure 1. Schematic of combustor and sampling system.

Cryogenic sampling was initiated when combustor operation had stabilized. Sample time was 90 minutes unless operation was suspended because of ice blockage. The nominal sampling time ranged from 39.2 to 90 minutes.

The cryogenic trapping system is shown schematically in Figure 2. The sample gas was passed into the first cylinder (maintained at 0°C with ice water), through a heated inlet into the second cylinder (maintained at -78°C with pulverized dry ice), and through the final cylinder (maintained at -175°C with liquid nitrogen), a needle valve for flow control, and a flow meter. The nominal flow was 500 cc/min at 21.1°C and 760. The flow was maintained by the pressure of the exhaust from the combustor. The compounds that will not be trapped and concentrated are those with sufficient vapor pressure at -175°C to remain in the gas being processed by the system.

The sample cylinders (Fig. 3) have a volume of 150 cc. Teflon and stainless steel are the only materials exposed to the components of the gas being sampled. Temperature of the -78°C and -175°C cylinders are monitored with installed thermocouples. In the -78°C trapping cylinder, a heated inlet tube minimizes the formation of an ice plug. The 175°C cylinder has a safety disk which will release pressure in excess of 1000 psig.

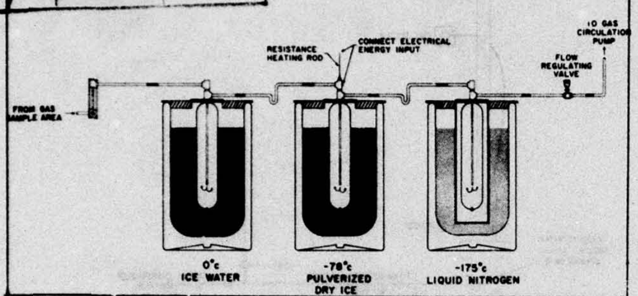

Figure 2. Flow diagram of multistage cryogenic sampling system.

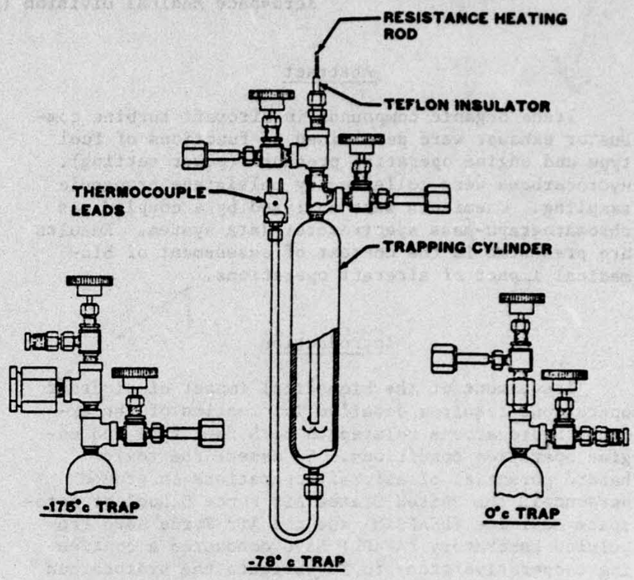

Figure 3. Diagram of trapping cylinder construction.

The cylinder in the liquid nitrogen bath (Fig. 4) is controlled at -175°C to prevent trapping liquid oxygen, which upon warming to room temperature could cause an overpressure condition. The cylinder is centrally suspended in a well surrounded by liquid nitrogen. A flow of warm dry gaseous nitrogen or helium from the bottom of the well controls the temperature of the cylinder.

In tests of the cryogenic trapping system with known concentrations of butane, the cryogenic system was 54.1% efficient in removing the compound. The combined cryogenic trapping and analysis systems produced an overall efficiency of 43%. The lower the vapor pressure of the material, the greater the overall recovery of a compound.

Analysis

Hydrocarbons in the samples were analyzed with a coupled gas chromatograph (Varian Model 1400) - mass spectrometer (DuPont Model 21-491) - data system (DuPont Model 21-094). The chromatographic column packing was Porapak Q (a polyalkyl styrene) of 100-120 mesh, in a 3-m long by 3-mm OD microbore (0.7 mm ID) stainless steel tube. This column, with temperature programming from -100°C to 250°C at approximately 10°C/min, has proven adequate for separating compounds ranging from methane to C_{10} aliphatic and aromatic hydrocarbons. The effluent from the chromatographic column was split 25% to a chromatographic flame ionization detector (FID), and 75% to the mass spectrometer jet separator, where helium is partially removed to enrich the contained organic compounds delivered to the mass spectrometer for identification. Compound quantitation was done by digital integration (Auto lab IV) of the chromatographic FID peak areas. Peak area/ppm is based on a 113 ppm hexane "Standard Lot, #020171R," prepared by Matheson Gas Products. Compound identification was provided by the MS-Data system using a DuPont Library Search program. The library is based on spectra of 23,879 compounds[6]. A laboratory concentration procedure in which the

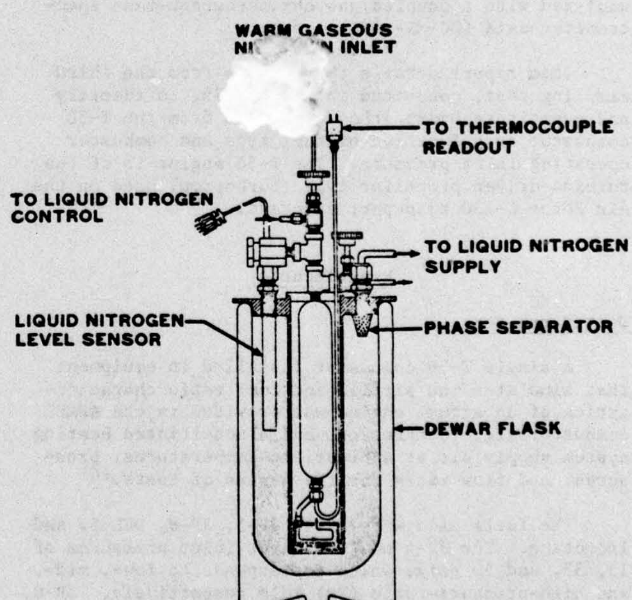

Figure 4. Diagram of liquid nitrogen trap.

sample from the cylinder (heated to 150°C) was passed through a GC sample loop (2.9 ml) held at liquid nitrogen temperature, was required because of the lack of hydrocarbon in most samples.

RESULTS AND DISCUSSION

There were 273 compounds reported in the samples from these tests. The compounds are listed in increasing molecular weight by chemical class in Tables

1, 3, and 5. There were 61 paraffins, 35 olefins, 3 diolefins, 16 naphthenes, 16 aromatics, 19 aldehydes, 35 alcohols, 22 ketones, 15 ethers, 13 esters, 14 nitrogen-containing compounds, 15 halogen-containing compounds, 4 sulfur-containing compounds, 1 silicon-containing compound, 3 lactones, and 1 organic peroxide.

To facilitate presentation and discussion of the results, the analyses are compiled in three distinct areas: 1) JP-4 fuel at increasing inlet pressures of 15, 33, and 50 psig; 2) the various fuels (JP-4, JP-5, JP-8, isooctane, and DEL-5 and duplicate samples at an inlet pressure of 33 psig; and 3) the JP-5 fuel, neat and with the ferrocene additive, at 75 psig.

JP-4 Fuel at 15, 33, and 50 psig Inlet Pressures

Table 1 lists the concentration of individual compounds associated with JP-4 at the various inlet pressures in ppm as hexane. It is of interest that the total hydrocarbon content compares favorably with the tests conducted in 1974.(2) Values of 22.6 ppm total hydrocarbon at 15 psig against 23.0 ppm in 1974, 3.7 ppm at 33 psig against 3.9 ppm in 1974, and .9 ppm at 50 psig against .7 ppm in 1974, indicate reproducibility with JP-4 fuel.

The combined data in Table 2 present the percent contribution by chemical class to the total hydrocarbon content. Paraffin content decreases slightly between 15 and 33 psig, and significantly at 50 psig, inlet pressure. The increasing inlet pressure of the combustor produces a greater percentage of oxygenated hydrocarbons (aldehydes, alcohols, ketones, ethers, and esters) at the expense of the unreacted components (paraffins, olefins, and diolefins). As in the earlier test, but not at the same combustor condition, β,β-dimethyl-propiolactone was identified with JP-4 fuel.

Various Fuels at 33 psig Inlet Pressure

Table 3 lists the compounds associated with the various fuels at 33 psig inlet pressure. The pure fuel (isooctane) indicates fewer species of paraffins than the other fuels. The olefins associated with this fuel are of lower molecular weight, and the only aromatic present was benzene. The DEL-5 duplicates agree well for total hydrocarbon content, but the isooctane duplicates are not consistent. The JP-8 value of total hydrocarbon 3.1 ppm as hexane compares favorably with the 1974 value of 4.4 ppm; however, the JP-5 value of 2.6 ppm is about 1/2 the value obtained in 1974 (5.3 ppm).

When presented as percent of the total hydrocarbon by chemical class, the data indicate many interesting trends (Table 4). The paraffins decrease as the aromatic content increases in the unburned fuels. Isooctane exhaust has the highest paraffin content; JP-4 exhaust, an intermediate content; and DEL-5, and JP-5, and JP-8, all high aromatic content fuels, the lowest paraffin content.

The olefin content is fairly consistent for isooctane, JP-4, and DEL, but increased with the higher boiling fuels, JP-5 and JP-8. The aromatic content is low with isooctane and is dramatically greater with DEL-5, which had 25% aromatic added to the JP-4 fuel. The highest concentrations of aldehydes and ketones were generated by the JP-5 and JP-8 fuels, with a concurrent decrease in paraffins. The highest concentration of nitrogen-containing compounds was distributed in JP-4 and DEL-5. The DEL-5 had nitrogen derivatives added to the JP-4 fuel.

Recent experimental findings indicate that if aromatic content increases, with a subsequent reduction in olefins, a decrease in PAN dosage occurs but eye irritation increases.(7) This indicates that DEL-5 would be the fuel likely to produce an eye discomfort when its exhaust products were added to the atmosphere. JP-5 and JP-8 with the substantial increase in olefins would be more likely to increase the PAN formation.

JP-5 and JP-5 + Ferrocene at 75 psig

Table 5 details the distribution of organic compounds in the tests with JP-5 and JP-5 + ferrocene. JP-5 fuel at the conditions of 75 psig inlet pressure produces low-molecular-weight paraffins the addition of ferrocene changes combustion characteristics, with a resulting increase in higher molecular weight species, as well as an increase in the total hydrocarbon. This increase, although not as dramatic, also occurs in the other chemical classes. Table 6 presents the data as percent of the total hydrocarbon content. As paraffins and olefins increase, ketones and aldehydes decrease. The increase in olefins, as a result of the ferrocene addition, may indicate greater PAN formation with the fuel additive.

While many of the oxygenates formed are likely the direct oxidation of the fuel, several other processes can produce the compounds. Methyl vinyl ether can be derived by the catalytic union of acetylene and methyl alcohol. Butyraldehyde maybe formed from propylene with carbon monoxide and hydrogen in the presence of a catalyst. Whereas the specific catalyst may not be present, the condition within the combustor may be sufficient to produce the same results.

SUMMARY AND CONCLUSIONS

Cryogenic sampling was used to sample hydrocarbon exhaust from a T-56 turbine engine combustor under conditions of low-, medium-, and high-PR idle as well as a high-power condition. Various fuels (isooctane, DEL-5, JP-4, JP-5, JP-5 + ferrocene, and JP-8) were burned. The principle conclusions from the study were:

1. Cryogenic sampling was an effective and reproducible technique for sampling gaseous hydrocarbon exhausts from turbine engines.

2. The hydrocarbon content of combustor exhaust was inversely related to operation pressure.

3. About 273 compounds were identified; of these, approximately half were aromatic and oxygenated species.

4. DEL-5 would possibly cause more eye discomfort but contribute less to PAN formation than JP-5 and JP-8.

5. Adding ferrocene to JP-5 results in an increase in gaseous hydrocarbons and in compounds which may be associated with PAN formation.

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TABLE 1. COMPOUNDS IDENTIFIED IN JP-4 FUEL EXHAUST AT VARIOUS INLET PRESSURES

	PRESSURE (psi)		
COMPOUND (ppm as hexane)	15	33	50
PARAFFINS	12.5	1.94	.103
Methane	0.015	0.0003	0.0098
Ethane	0.0028	0.017	0.0006
Propane	0.0004*	0.0010	0.0014
n-Pentane	0.62		
2-Methyl Pentane	0.26		
n-Hexane	0.57	0.053	
2,2,3-Trimethyl Butane		0.024	
3-Methyl Hexane	1.9	0.33	
2,3-Dimethyl Pentane			0.013
n-Heptane	0.99	0.15	
2,3,3-Trimethyl Pentane	2.3	0.0031	0.010
2,4-Dimethyl Hexane	0.25	0.12	0.032
3,3-Dimethyl Hexane	0.057	0.094	0.0060
n-Octane	1.7		0.0030
2,2,3,3-Tetramethyl Pentane	0.43	0.046	
2,2,3,4-Tetramethyl Pentane		0.33	0.0056
2,3-Dimethyl-3-Ethyl Pentane	0.11		
2,3,4-Trimethyl Hexane	0.45	0.18	
2-Methyl-4-Ethyl Hexane	0.68	0.19	
2,2-Dimethyl Heptane		0.068	
2,4-Dimethyl Heptane			0.0021
2,5-Dimethyl Heptane	0.35		0.0056
3,4-Dimethyl Heptane	0.38		
3-Methyl Octane	T		
4-Methyl Octane		T	
n-Nonane	1.0	0.21	0.014
4-Methyl-5-Ethyl Heptane	0.16		
2,3-Dimethyl Octane	0.043	0.064	
2,6-Dimethyl Octane	0.010		
4,5-Dimethyl Nonane		0.064	
4-Methyl Decane	0.035		
n-Undecane	0.19		
OLEFINS	4.37	0.245	0.077
Acetylene	0.38	0.063	0.0011
Ethene	0.59	0.0009	0.022
Propene	1.5	0.040	0.0099
2-Methyl Propene	0.022	0.0026	
1-Butene	0.013	0.013	0.0066
2-Butene	0.088		
2-Methyl-1-Butene		0.0094	
2-Methyl-2-Butene	0.11		

(TABLE 1 continued)

1-Pentene	0.56	0.011	0.016
2-Pentene-cis	0.11		
2-Methyl-1-Pentene	0.31		0.0030
4-Methyl-1-Pentene	0.15		
3-Methyl-cis-2-Pentene			0.0010
1-Hexene			0.0075
Unknown (5-Methyl-1-Hexyne)			0.0017
2-Methyl-trans-3-Hexene			0.0085
4-Methyl-1-Hexene	0.54	0.10	
DIOLEFINS	0.12	0.0083	0.0008
Allene	0.12	0.0005	0.0008
Isoprene		0.0078	
NAPHTHENES	0.54	0.073	
Ethyl Cyclobutane		0.0008	
Dimethyl Cyclopentane	0.54		
Methyl Cyclohexane		0.072	
AROMATICS	2.09	0.676	0.077
Benzene	0.51	0.18	0.035
Toluene	0.65	0.16	0.025
Unknown (m-Xylene)	0.91	0.092*	
p-Xylene		0.15	0.017
n-Propyl Benzene		0.094*	
m-Diethyl Benzene	0.019		
ALDEHYDES	1.63	0.262	0.138
Acetaldehyde	0.42	0.18	0.093
Acrolein	0.064	0.0087	0.0002
Propanal	0.040	0.0020	
Glycoladehyde	0.0035		T
n-Butanal	0.068	0.0081	0.022
2-Butanal		0.0084	
Crotonaldehyde	0.62	0.031	0.015
m-Valeraldehyde	0.057	0.017	0.0060
n-Hexanal		0.0035	0.0022
Unknown (2,4-Dimethyl Pentanal)		0.0034	
ALCOHOLS	0.0279	0.0368	0.0695
Methanol	0.0042	0.011	0.028
Allyl Alcohol	0.0046		
4-Pentene-1-ol	T	0.016	
3-Methyl-1-Butanol		0.0096	0.0069
3-Methyl-3-Butene-2-ol			0.032
3-Methyl-1,2-Cyclopentanediol			0.0026
1-Heptanol		0.0002	
Unknown (2,24-Trimethyl-3-Pentene-1-ol)	0.0039		
2-Ethyl Hexanol-1	0.0082		
Unknown (2,6-DI-tert-Butyl Hydroquinone)	0.0070		
KETONES	0.767	0.257	0.0876
Acetone	0.40	0.19	0.068
Methyl Vinyl Ketone	0.31	0.037	0.0013
Methyl Propyl Ketone	0.057	0.034	0.0037
Methyl Isobutyl Ketone		T	0.0008
2-Methyl-3-Pentanone			0.013
ETHERS	0.12	0.066	T
Vinyl Methyl Ether			T
Ethyl Vinyl Ether	0.12	0.066	
ESTERS	0.019	0.0016	0.0016
Methyl Formate		0.0016	
Isobutyl Formate	0.019		
Unknown (β-Phenyl Ethyl Isobutanoate)			0.0016
NITROGEN-CONTAINING	0.0319	0.0743	0.0328
Methyl Cyanide	0.014	0.073	0.0048
Glycolonitrile			0.0010
Nitromethane	0.0049		0.0028
Imidazole	0.013		

(TABLE 1 continued)

n-Valeronitrile			0.0002
neo-Pentyl Nitrate			0.024
β-Keto-1-Nitro-Octane		0.0003	
HALOGEN-CONTAINING	0.389	0.0171	0.0070
Chloromethane			T
n-Butyl Fluoride			0.0010
1-Fluorobutane	0.16	0.0011	
Unknown (2-Chlorobutane)	0.22		
Methyl Bromide	0.0008		
Cyclohexyl Fluoride		0.0016	
2-Chloro-3-Methyl Butane	0.0082		
Amyl-2,2-Dichloropropionate			0.0060
SULFUR-CONTAINING	0.0087		
2-Methyl-1-Pentanethiol	0.0087		
SILICON-CONTAINING	0.0091		
Methyl Silane	0.0091		
LACTONES		0.0006	
ββ-Dimethyl Propiolactone		0.0006	

*Identified by gas chromatography.

TABLE 2. PERCENT OF JP-4 FUEL EXHAUST AT VARIOUS INLET PRESSURES

Compound class	JP-4 15 PSIG	JP-4 33 PSIG	JP-4 50 PSIG
Paraffins	55.3	53.0	17.2
Olefins	19.3	6.7	12.9
Diolefins	0.5	0.21	<.1
Naphtheses	2.4	2.0	
Aromatics	9.2	18.5	12.9
Aldehydes	7.2	7.2	23.6
Alcohols	0.1	1.0	11.7
Ketones	3.4	7.0	14.6
Ethers	0.5	1.8	
Esters	<.1	<.1	0.3
Nitrogen-containing	0.1	2.0	5.5
Halogen-containing	1.7	0.5	1.1
Sulfur-containing	<.1		
Silicon-containing	<.1		
Lactones		<.1	

TABLE 3. COMPOUNDS IDENTIFIED IN VARIOUS FUEL EXHAUSTS AT 33 PSIG

COMPOUND (ppm as hexane)	ISOOCTANE	ISOOCTANE	JP-4	DEL-5	DEL-5	JP-5	JP-8
PARAFFINS	.418	1.41	1.94	.644	.466	.204	.621
Methane	0.0098	0.0170	0.0003	0.0084	.011	0.0052	.014
Ethane	0.0011	0.0021	0.017	0.0027	0.0008	0.0007	0.0034
Propane			0.0010	0.0002			
2-Methyl Propane					0.0003		
n-Pentane	0.0049						
n-Hexane		0.0089	.053	0.0010	0.011		
2,2,3-Trimethyl Butane			0.0240	0.0056			
2-Methyl Hexane				.096			0.11
3-Methyl Hexane			0.33	0.019	0.094		
n-Heptane			0.15	0.057	0.012		
2,2,3,3-Tetramethyl Butane		0.91					
2,2,3-Trimethyl Pentane				0.029			0.0025
2,3,3-Trimethyl Pentane			0.0031				
2,2,4-Trimethyl Pentane	0.40	0.40		0.089	0.061		
2,2-Dimethyl Hexane		0.075					
2,4-Dimethyl Hexane			0.121	0.065	0.087	0.0040	
3,3-Dimethyl Hexane			0.094	0.0051			
Unknown (2-Methyl Heptane)							0.019
n-Octane			0.046	0.071	0.015		
2,2,3,3-Tetramethyl Pentane			0.33				
2,2,3,4-Tetramethyl Pentane							0.023

(TABLE 3 continued)

2,2,5-Trimethyl Hexane							0.025
2,3,4-Trimethyl Hexane			0.18	0.0084	0.013		
2,3,5-Trimethyl Hexane							0.0042
2-Methyl-4-Ethyl Hexane			0.19			0.0490	0.038
2,5-Dimethyl Heptane				T			
2,2-Dimethyl Heptane			0.068				
3,3,-Dimethyl Heptane							0.013
3,4-Dimethyl Heptane	0.0017	0.0019			0.016		
3-Ethyl Heptane						0.027	
4-Ethyl Heptane					0.0065		
4-Methyl Octane					0.011		0.0310
n-Nonane			0.21	0.089	0.060	0.096	0.080
2,3-Dimethyl Octane			0.064				
2-Methyl-5-Ethyl Heptane							0.0058
2-Methyl Nonane					0.028		
n-Decane				0.024	0.016		0.050
2,3,4-Trimethyl Octane				0.011			
3,3,5-Trimethyl Octane					0.0011		
2,5-Dimethyl Nonane							0.070
4,5-Dimethyl Nonane			0.064				
3-Methyl Decane				0.063			
Unknown (1-Phenyl-2-Ethyl Butane)							0.096
Unknown (1-Phyenyl-2,4-Dimethyl Pentane)					0.0021		
n-Tridecane						0.016	
Unknown(1,3-Dicyclohexyl-2-Methyl Propane)							0.0036
Unknown(2-Phenyl-4,4-Dimethyl Decane							0.032
Unknown(2-Penyl-Pentadecane						0.0060	
OLEFINS	0.0540	.219	.0249	.237	.218	.649	1.05
Acetylene	0.039	0.016	.068	.050	0.0032	0.0012	0.044
Ethene	0.0027	0.0063	0.0009	0.086	0.085	0.027	0.11
Propyne		0.025				0.0064	
Propene	0.0013	0.11	0.040	0.050	0.060	0.22	0.51
2-Methyl Propene		0.011	0.0026		0.0001		
1-Butene		0.0028	0.013	0.016	0.0053	0.071	0.0053
2-Butene					0.0002		
1-Pentyne						0.027	
Unknown(3-Methyl-1-Butene)						0.011	
2-Methyl-1-Butene			0.0094				
1-Pentene		0.0001	0.011	0.0074	0.0034	0.0048	0.0083
2-Pentene-cis						0.0040	
Unknown(3-Hexyne)						0.0007	
4-Methyl-1-Pentene		T					0.013
2-Methyl-trans-2-Pentene				0.0047			
1-Hexene				0.018	0.030	0.11	0.073
2,3,3-Trimethyl-1-Butene		0.016					
4,4-Dimethyl-1-Pentene					0.0016		
2,4-Dimethyl-2-Pentene	0.011						
4,4-Dimethyl-trans-2-Pentene		0.033					
2-Methyl-1-Hexene							0.0190
4-Methyl-1-Hexene			0.10	0.0049			
1-Heptene						0.14	0.16
trans-3-Heptene					0.030		
1-Octene						0.0010	0.071*
2,6-Dimethyl-3-Heptene						0.025	
1-Nonene							0.014
2,6-Dimethyl-1-Octene							0.031
DIOLEFINS	0.0017		0.0083	0.0059	0.0003		0.046
Allene	0.0017		0.0005	0.0007	0.0003		0.041
Isoprene			0.0078	0.0020			0.0047
2,4-Hexadiyne				0.0032			
NAPHTHALENES		T	.0728	.0570	0.025	0.121	0.105
Unknown(Cyclobutane)		T					
trans-1,2-Dimethyl Cyclopropane						0.019	
Cyclopentane							0.0076
Cyclohexane							0.011
Ethyl Cyclobutane			0.0008				
1-Methyl-1-Ethyl-Cyclopropane				0.012		0.012	
Isopropyl Cyclopropane						0.0043	
1,1-Dimethyl Cyclopentane						0.068	
trans-1,3-Dimethyl Cyclopentane						0.018	
Methyl Cyclohexane			0.072				
6,6-Dimethyl fulvene				0.045	0.025		

(TABLE 3 continued)

1-cis-2-cis-3-Trimethyl Cyclopentane							0.085
n-Butyl Cyclohexane							0.0004
AROMATICS	0.0091	0.024	0.681	1.48	1.42	0.451	0.37
Benzene	0.0091	0.024	0.185	0.082	0.0748	0.26	0.17
Toluene			0.16		0.785	0.11	0.11
Unknown(m-Xylene)			0.092*		0.1152	0.058	
O-Xylene				0.16	0.0247		
p-Xylene			0.15	0.75	0.1074	0.023*	0.30
1,2,3-Trimethyl Benzene				0.030	0.0065		
1,3,5-Trimethyl Benzene				0.069			
Unknown(1-Methyl-2-Ethyl Benzene)					0.0102		
1-Methyl-3-Ethyl Benzene				T	0.0956		
Isopropyl Benzene				0.12	0.0828		
Unknown(n-Propyl Benzene)							0.038
n-Propyl Benzene			0.092*	0.15	0.1159		
Unknown(1,2-Dimethyl-4-Ethyl Benzene)				0.0073			
m-Diethyl Benzene				0.0073	0.0033		
Isobutyl Benzene							0.022
Unknown(o-Ethyl Toluene)				0.0092			
p-Ethyl Toluene				0.016			
ALDEHYDES	0.0631	0.145	0.260	0.134	0.185	0.502	0.331
Acetaldehyde	0.021	0.038	0.18	0.096	0.10	0.22	0.18
Acrolein	0.0007	0.0003	0.0087	0.0019	0.0049	0.0009	0.011
Propanal						0.0023	0.014
Glycolaldehyde					0.0009		
Crotonaldehyde	0.014	0.011	0.031	0.012	0.041	0.015	0.036
n-Butanal	0.032	0.0080	0.0081	0.0058	0.0076	0.15	0.047
2-Butanal(2-Methyl Propanal)		0.0087	0.0084				
Trimethyl Acetaldehyde	0.021						
2-Methyl Butanal		0.066		T			
m-Valeraldehyde(n-[illegible])		0.002	0.017			0.084	0.025
n-Hexanal	0.0032	0.011	0.0035	0.0074		0.016	0.0072
Benzaldehyde							0.0061*
n-Heptaldehyde				0.0019	0.031		0.0051
Unknown(2,4-Dimethyl Pentanal)			0.0034				
P-Tolualdehyde				0.0072			
Unknown(trans-2-Octanal)							T
Unknown(2-Phenyl Propanal)				0.0014			
ALCOHOLS	0.0047	0.189	0.0368	0.0451	0.100	0.171	0.118
Methanol	0.001	0.14	0.011	0.0048	0.01	0.023	0.0021
Ethanol						0.0002	0.0012
1-Propen-3-ol					0.0009		
2-Methyl Propanol					0.0075		
2-Buten-1-ol					0.033		
cis-2-Buten-1-ol							0.0010
1-Butanol				0.0008	0.0006		
2-Methyl-2-Propanol		0.029					
2,4-Hexadiene-1-ol	0.0017						T
3-Methyl-1-Butanol			0.0096	0.0019			
3-Methyl-2-Buten-1-ol							0.0013
4-Pentene-1-ol			0.016				
Unknown(Methyl Butanol)		0.0013					
3-Butene-1,2-diol					0.0050		
trans-2-Hexene-1-ol	0.0020						
Cyclo Hexanol				0.0067	0.015		
2-Methyl-1-Pentanol				0.0062	0.020		
3-Methyl-1-Pentanol				0.0005	0.0020	0.030	
1-Hexyn-3-ol		0.01					
Cyclohexane Methanol				0.017			0.014
1-Heptanol			0.0002			0.023	
2-Heptanol				0.0060			
Unknown(3-Octene-1-ol)							0.0016
2-Ethyl Hexanol-1		0.0027			0.0061	0.051	0.097
1-Octanol						0.0440	0.084
Dimethyl-2,5-Hexanediol		0.0059					
2-Propyl Heptanol							T
Unknown(6-Ethyl-3-Octanol)		T					
1-Decanol				0.0012			
KETONES	0.105	0.153	0.261	0.191	0.288	0.389	0.329
Acetone	0.089	0.14	0.19	0.12	0.20	0.23	0.17
Methyl Vinyl Ketone		0.0002	0.037	0.0030	0.0015	0.016	0.0059

(TABLE 3 continued)

Methyl Ethyl Ketone					0.019		
Methyl Propyl Ketone	0.0012	0.0008*	0.034	0.031	0.017		0.032
5-Hexen-2-one	0.0028						
Ethyl Propyl Ketone		0.0011			0.051		
Methyl Isobutyl Ketone		0.0002		0.0080		0.0022*	0.0098
Unknown(Phenyl Methyl Ketone)					T		
4,4-Dimethyl-2-Pentanone	0.012	0.011					
Unknown(2-Methyl-3-Heptanone)							0.038
Unknown(4-Methyl-2-Heptanone)						0.0061	
Cyclopentanone						0.03	
2-Methyl Cyclooctanone							0.04
2,2,5-Trimethyl Hexane-3,4-dione							0.018
Unknown(2,2,5-Trimethyl Hexane-3,4-dione)				0.0291			
Unknown(Propyl Benzyl Ketone)							0.0068
Unknown(Isopropyl Benzyl Ketone)						0.039	0.0024
Unknown(Undecanone)							0.0029
ETHERS	0.0144	0.0664	0.066	0.0499	0.0193	0.0205	0.0761
1-2-Epoxy Propane			0.0005				
Vinyl Methyl Ether		0.0001			T		
Trans-2,3-Epoxy Butane				0.017			0.0011
2,3-Epoxy Butane		0.0033					
Ethyl Vinyl Ether			0.066	0.026	0.019		0.040
2-Methyl Tetrahydrofuran							0.035
Allyl Ether				0.0040			
3-Isopropyl Oxetane					0.0002		
Isobutyl BVinyl Ether	0.0076						
n-Butyl Vinyl Ether						0.0085	
Hexyl Vinyl Ether					0.0001		
2,2,4,4-Tetramethyl Tedrahydrofuran	0.0068	0.063					
Unknown(1-Methoxy-Phenyl Ethane)						0.012	
Benzyl Ether				0.0024			
Octadecyl Vinyl Ether							T
ESTERS		0.0071	0.0016	0.0017		0.0311	0.0032
Methyl Formate			0.0016				
Unknown(Ethyl Formate)						0.0071	
Unknown(n-Butyl Formate)						0.0050	
Allyl Propionate		0.0024					
Unknown(1-Methyl Butyl Propionate)				0.0017			
n-Heptyl Acetate						0.019	
Octyl Acetate		0.0047					
Unknown(Sec-Octyl Acetate)							0.0032
Unknown(p-tert-Butylphenoxylmethyl Acetate)		T					
NITROGEN CONTAINING	0.0050	0.0103	0.0743	0.0374	0.0407		0.0119
Methyl Cyanide		0.0026	0.073	0.0021	0.0021		0.0021
Unknown(Ethyl Cyanide)				0.0009			
Nitro Methane	0.0050	0.0034		0.011	0.017		0.0086
Inidazole				0.021			
Unknown(Pyrazole)					0.0026		
Unknown(2-Ethyl-1-Diazridine)							0.0012
Unknown(Valeronitrile)				T			
2,4-Dimethyl Inidazoline					0.019		
3,6-Dipropyl-1,2,4,5-Tetrazine				0.0024			
β-Keto-1-Nitro-Octane		0.0043	0.0013				
HALOGEN CONTAINING	0.019		0.0171	0.0023	T		
4-Chloro-2-Methyl Butane	0.0078			0.0023			
1-Flurobutane			0.0011				
1,2-Dchloropropane	0.0046						
Cyclohexyl Fluoride			0.016				
1-Fluoroheptane				T			
Trichloroethylene	0.0066						
SULFUR CONTAINING				T	0.046		T
Carbon Disulfide				T			
2-Methyl-1-Pentanethiol				T	0.046		
Octyl Mercaptan							T
LACTONES			0.0006	T		0.0065	
ββ-Dimethyl Propiulactone			0.0006			0.0065	
γ-Capro Lactone				T			
Unknown(α-Acetyl Butyro Lactone)				T			

(TABLE 3 continued)

PEROXIDES	0.0023
Dimethyl Peroxide	0.0023

*Identified by gas chromatography.

TABLE 4. PERCENT OF VARIOUS FUEL EXHAUSTS AT 33 PSIG INLET PRESSURE

Compound	Isooctane	Isooctane	JP-4	DEL-5	DEL-5	JP-5	JP-8
Paraffins	60.2	63.4	53.0	22.3	16.0	8.0	20.3
Olefins	7.8	9.8	6.7	8.2	7.8	25.5	34.3
Diolefins	0.2		0.2	0.2	<.1		1.5
Naphthalenes			2.0	2.0	0.9	4.8	3.4
Aromatics	1.3	1.1	18.5	51.3	50.9	17.7	12.1
Aldehydes	9.1	6.5	7.2	4.6	6.6	19.7	10.8
Alcohols	0.7	8.5	1.0	1.5	3.6	6.7	3.9
Ketones	15.1	6.9	7.0	6.6	10.3	15.3	10.7
Ethers	2.1	3.0	1.8	1.7	0.7	0.8	2.5
Esters		0.3	<.1	<.1		1.2	0.1
Nitrogen-containing	0.7	0.5	2.0	1.3	1.5		0.4
Halogen-containing	2.7		0.5	<.1			
Sulfur-containing					1.6		
Lactones			<.1			0.3	
Peroxides				<.1			

TABLE 5. COMPOUNDS IDENTIFIED IN FERROCENE (Fe) FUEL EXHAUST AT 75 PSIG INLET PRESSURE

COMPOUND (ppm as hexane)	No Fuel	JP-5	JP-5†	JP-5	JP-5 + Fe	JP-5 + Fe
PARAFFINS	0.0373	T	0.0002	0.0011	0.173	0.0602
Methane	0.0002		0.0002	0.0001		
Ethane	0.0004			T		
Propane	0.0006	T	T	0.0010		
n-Butane	0.0016					
2-Methyl Propane	0.0003					
2,2-Dimethyl Propane				0.0002*	0.0268	
2-Methyl Butane	0.015					
n-Pentane	0.0006					
2-Methyl Pentane	0.0007					
n-Hexane	0.0005			0.10		
2,3-Dimethyl Pentane	0.0067				0.0099*	T
n-Heptane	0.0020*				0.0621	0.0056
2,3,4-Trimethyl Hexane	T*					0.0092
3-Methyl-4-Ethyl Hexane						0.0092
2,4-Dimethyl Heptane					0.0002	
3,4-Dimethyl Heptane					0.0005	
4-Ethyl Heptane						T
n-Nonane	0.0029					0.0073
2,2-Dimethyl-4-Ethyl Hexane						0.0021
Unknown (2,7-Dimethyl Octane)	0.0054					
OLEFINS	0.0027	0.0006	0.0141	0.0057	0.038	0.0707
Acetylene	0.0001			T		
Ethene	0.0002					
Propene	0.0005	0.0001	0.0005	0.0021	T	0.0004
2-Methyl Propene	0.0009		0.0011	0.0022	0.0003	0.0015
1-Butene		0.0005	0.0001	0.0014		0.069
2,4-Dimethyl-1-Pentene				0.038		
2-Methyl-1-Hexene	0.0010					
2,4,4-Trimethyl-1-Pentene			0.012			
NAPHTHENES					0.0258	
Cyclohexane					0.0028	
Methyl Cyclohexane					0.023	
AROMATICS	0.0113	0.0101	0.0191	0.0069	0.101	0.047
Benzene	0.0022	0.0095	0.012	0.0069	0.069	0.035
Toluene	0.0070	0.0006	0.0071		0.032	0.012
Unknown (m-Xylene)	0.0001					
o-Xylene	0.0020					
p-Xylene					0.0003*	0.0138

(TABLE 5 continued)

ALDEHYDES	0.0110	0.0306	0.0227	0.0294	0.0107	0.213
Acetaldehyde	0.0034	0.019	0.014	0.028	0.0086	0.12
Acrolein		0.0002			T	0.0011
Propanal					0.0006	
Glycoladehyde		0.0012				
n-Butanal	0.0005		0.0025	0.0014	0.0005	0.058
2-Butanal (2-Methyl Propanal)						0.0012
2-Methyl Butanal		0.0002	0.0062			
m-Valeraldehyde (n-Pentanal)					0.0006	0.023
Unknown (Iso Valeraldehyde)	0.0071					
n-hexanal					0.0004	0.0093
n-Heptaldehyde						0.0001
ALCOHOLS	0.0010	0.0081	0.0044	0.0093	0.0016	0.184
Methanol		0.0014	0.0020	T	T	0.0040
2-Methyl-2-Propanol	0.0010	0.0059	0.0024	0.0093	0.0016	0.180
3-Pentanol		0.0008				
KETONES	0.0048	0.0216	0.0173	0.0306	0.0076	0.211
Acetone	0.0041	0.017	0.015	0.027	0.0076	0.20
Methyl Ethyl Ketone		0.0046				
Methyl Propyl Ketone			0.0023	0.0036		0.011
Unknown (4-Methyl Cyclohexanone)	0.0007					
Methyl Isopropyl Ketone	T					0.0003
Methyl Isobutyl Ketone						0.0038
3-Heptanone						T
Unknown (Isopropyl Benzyl Ketone)						0.0021
ETHERS			0.0049	0.0058	0.0005	
trans-2,3-Epoxy Butane					T*	
Ethyl Vinyl Ether				0.0049	0.005[illegible]	0.0005
ESTERS	0.0017					T
Unknown (Amyl Formate)						T
Unknown (2-Methyl Butyl Isopentanoate)	0.0017					
NITROGEN-CONTAINING	T	0.0020	0.0018	0.0084	0.0008	0.039
Methyl Cyanide		0.0006*	0.0015*			0.0004
Unknown (Propane Nitrile)		T				
Nitromethane	T	0.0007	0.0003	0.0003	0.0008	0.035
2-Methyl-2-Nitropropane		0.0007		0.0081		
HALOGEN-CONTAINING	0.0081	0.0013	0.0045	0.013	T	0.037
Chloromethane		T			T*	0.0012
1-Chloro-3-Methyl Butane	T					
Unknown (1-Chlorohexane)					T*	0.0008
Trichloroethylene	0.0068	0.0013	0.0014	0.013		0.035
R-113	0.0013		0.0031			
SULFUR-CONTAINING				0.0016		0.0056
Unknown (Isopropyl Butyl Sufide)				0.0016		
n-Octyl Mercaptan						0.0056

*Identified by gas chromatography.

TABLE 6. PERCENT OF JP-5 AND JP-5 + FE JET EXHAUST AT 75 PSIG INLET PRESSURE

Compound	No fuel	JP-5	JP-5	JP-5 + FE	JP-5 + FE
Paraffins	47.9	1.0	48.1	6.9	
Olefins	3.5	0.8	5.1	10.7	8.2
Naphthenes				7.2	
Aromatics	14.5	13.6	6.2	28.1	5.4
Aldehydes	14.1	41.2	26.3	3.0	24.6
Alcohols	1.3	10.9	8.3	0.4	21.2
Ketones	6.2	29.1	27.4	2.1	24.3
Ethers			5.2	0.1	
Esters	2.2				<.1
Nitrogen-containing		3.1	7.5	0.2	4.5
Halogen-containing	10.4	2.0	11.6		4.3
Sulfur-containing			1.4		0.6